

Effect of Local Inhomogeneity on Nucleation; Case of Charge Density Wave Depinning

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(Received)

The spatial inhomogeneities are expected to affect nucleation process in an essential way. These effects are studied theoretically by considering the case of the depinning of the charge density wave as a typical example. The threshold field of the depinning of the one-dimensional commensurate charge density wave with one impurity has been examined based on the phase Hamiltonian at absolute zero. It is found that the threshold field is lowered by a finite amount compared to that in the absence of an impurity.

KEYWORDS: nucleation, inhomogeneity, frustration, charge density wave (CDW), commensurability, impurity, threshold field, phase Hamiltonian

§1. Introduction

Nucleation is one of the most drastic phenomenon in various fields of physics, chemistry, biology, and also in engineering.¹⁾ Especially, the nucleation in condensed matter physics is most interesting in the sense that it can be controlled by such parameters as pressure, temperature, electric and magnetic fields so on. In general nucleation is defined as a phenomenon where a new phase appears locally in space.

The theoretical analysis of nucleation was given by Langer,²⁾ who investigated the problem of reversing of the direction of magnetization in a ferromagnetic system. In the process of reversing, changes of magnetization is found to be not uniform in space but it is triggered by the appearance of the magnetic bubbles called droplets. While this theory offers the fundamental understanding of the nucleation in a homogeneous medium, we know that a local inhomogeneity in actual systems plays important roles in the nucleation process, which will be studied in this paper. For explicit studies we choose the case of the charge density wave (CDW)³⁾ depinning as a typical example, because the field theory which is described by the phase Hamiltonian has been established,⁴⁾ and

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the concept of the nucleation can be defined clearly in this case as the appearance of the spatially local non-uniform structure of the phase variable which triggers the depinning.

CDW is one of the characteristic state of quasi-one-dimensional conductors, where translational symmetry is spontaneously broken. The gapless sliding mode⁵⁾ that incarnates Goldstone mode can be pinned by the external objects which break the translational symmetry. If the external object is the underlying lattice whose spatial periodicity is commensurate to CDW's, it is called commensurate CDW. In this case CDW behaves as an insulator. However, if electric field is applied, CDW starts to move above some critical field called threshold field. To estimate the threshold field theoretically, the phase Hamiltonian approach⁶⁾ is useful. With the phase Hamiltonian approach, the classical threshold field can be derived as the field at which the potential barrier for the sliding disappears. In this paper we investigate classically the depinning processes of one-dimensional commensurate CDW with inhomogeneity at absolute zero.

In §2 we introduce our model based on the phase Hamiltonian. In §3 we review briefly in a homogeneous case. Below the uniform depinning field, the nucleation requires a finite excitation energy. In §4 we examine the ground state in the presence of an impurity and in §5 we investigate the threshold field in this case. The threshold field can be smaller than the uniform depinning field and depinning sets at the impurity site. In §6 the potential curve of our model is shown. Our conclusion and discussion are given in §7. The effects of three dimensionality and fluctuations, quantum and thermal, will be studied separately.

§2. The Model

We investigate the one-dimensional commensurate CDW with one impurity located at X_i . The Lagrangian is then given by

$$\mathcal{L} = - \int dX \left[A \left(\frac{\partial \phi}{\partial X} \right)^2 - F\phi + g(1 - \cos(M\phi)) - V_i \cos(2k_F X + \phi) \delta(X - X_i) \right]. \quad (2.1)$$

Here, the first term in the integration is the elastic energy, $A = (\hbar v_F)/(4\pi)$, with v_F being the Fermi velocity. The second term is the energy associated with the electric field, $F = (eE)/(2\pi)$, with E and $-e$ ($e > 0$) being electric field and the electron charge, respectively. The third term is the commensurability energy, $g = (|\Delta|^2/\varepsilon_F)n_e(|\Delta|/W)^{M-2}$, $|\Delta|$ being the Peierls gap, and ε_F , n_e , W are the Fermi energy, the density of electron, and the width of the original band, respectively. Here M is the degree of commensurability, $M = \pi/(k_F a)$, k_F is the Fermi wave number, a is the lattice spacing. The last term is the coupling energy of CDW to one impurity. In this Lagrangian, there exists a characteristic length, $\xi = \sqrt{(2A)/(M^2 g)}$, which is the phase coherence length due to the commensurability. We make the Lagrangian dimensionless through scaling by this ξ ; i.e. $x = X/\xi$, $\mathcal{L} = M^2 g \xi L$, where L is given by

$$L = - \int dx \left[\frac{1}{2} \left(\frac{\partial \phi}{\partial x} \right)^2 - \varepsilon \phi + \frac{1}{M^2} (1 - \cos(M\phi)) - v \cos(\chi + \phi) \delta(x - x_i) \right]. \quad (2.2)$$

Here $\varepsilon = F/(gM^2)$, $v = V_i/(g\xi M^2)$. In this paper, we assume $\varepsilon \geq 0$. Further, we define $x_i = X_i/\xi$ and $\chi = (2\pi z)/M$, where $z = X_i/a$ characterizes the location of an impurity relative to the site where the energy gain by commensurability is maximum. The range of χ is $-\pi/M \leq \chi \leq \pi/M$, because the Lagrangian has the periodicity of $2\pi/M$ with respect to the phase.

§3. The Homogeneous Case

First of all, we examine the case of $v = 0$, namely the homogeneous case.⁷⁾

The stable configuration of the phase is determined by varying Lagrangian;

$$-\phi'' - \varepsilon + \frac{1}{M} \sin(M\phi) = 0. \quad (3.1)$$

When $\varepsilon = 0$, eq. (3.1) is the sine-Gordon equation, and has two kinds of solutions, which are a trivial one, $\phi = 0$, and the kink solution, which is given by

$$\phi(x) = \frac{4}{M} \arctan [\exp(\pm(x - x_0))] \equiv \phi_{\pm}(x - x_0), \quad (3.2)$$

and shown in Fig. 1. Here x_0 is the center of the kink. Among these solutions, the lowest energy

Fig. 1. The classical solution in the case of $\varepsilon = 0$. The solid line is a kink and the dotted line is an anti-kink.

solution, namely, the ground state solution is $\phi = 0$, and the kink and the anti-kink are excitations with finite excitation energy.

In the case of $\varepsilon \neq 0$ the equation of the classical configuration has also an uniform solution,

$$\phi = \frac{1}{M} \arcsin(\varepsilon M), \quad (3.3)$$

and the non-uniform solution with local spatial variation, $\phi_l(x)$, which is given by

$$\phi_l' = - \left[2 \left[\varepsilon \left(\frac{1}{M} \arcsin(\varepsilon M) - \phi_l \right) + \frac{1}{M^2} \left(\sqrt{1 - (\varepsilon M)^2} - \cos(M\phi_l) \right) \right] \right]^{\frac{1}{2}}. \quad (3.4)$$

This equation is derived by the integration of eq. (3.1) with the boundary condition, $\phi(\infty) = (1/M) \arcsin(\varepsilon M)$ and $\phi'(\infty) = 0$. The solution, $\phi_l(x)$, is shown in Fig. 2. We notice that the non-uniform solution, $\phi_l(x)$, is kink pair solution.

Fig. 2. The non-uniform solution, $\phi_l(x)$, of the classical equation in the case of $\varepsilon = 0.1$.

In the presence of the electric field, the cosine-type potential for the uniform phase is tilted as is shown in Fig. 3. The potential barrier disappears at $\varepsilon = 1/M \equiv \varepsilon_T$, which is the classical depinning field of the uniform CDW.

On the other hand, if the kink pair is excited, CDW will also depin. This is another type of depinning process which sets locally in space and considered to be the nucleation process. However, below the threshold field, ε_T , of the uniform depinning, the kink pair is always the excitation, which requires a finite excitation energy. Therefore the nucleation does not take place in a homogeneous case without quantum nor thermal fluctuations.

§4. Ground State in the Presence of an Impurity

Next, we consider a case with an impurity, $v \neq 0$. The stable configuration of the phase is now given by

$$-\phi'' - \varepsilon + \frac{1}{M} \sin(M\phi) + v \sin(\chi + \phi) \delta(x - x_i) = 0, \quad (4.1)$$

Fig. 3. The potential for the uniform phase at $\varepsilon = 0.1$ for a choice of $M = 4$.

with the boundary conditions

$$\phi(\pm\infty) = \frac{1}{M} \arcsin(\varepsilon M), \quad \phi'(\pm\infty) = 0. \quad (4.2)$$

In the case of $\varepsilon = 0$, the solution is given analytically. Depending on the range of χ , there are two kinds of configurations. If χ is in the range of $-\pi/M \leq \chi \leq 0$, the solution is located in the region between 0 and π/M (Config.1) as shown in Fig. 4. If χ is in the range of $0 \leq \chi \leq \pi/M$, the solution is located in the region between $-\pi/M$ and 0 (Config.2). We take electric field $\varepsilon \geq 0$. Under this condition, Config.1 has more tendency to depin than Config.2. Namely, in the case of $-\pi/M \leq \chi \leq 0$, the threshold field can be smaller than that of uniform depinning as is disclosed in §5; in the case of $0 \leq \chi \leq \pi/M$, however, the threshold field is same as that of uniform depinning. Therefore, we consider only the case of $-\pi/M \leq \chi \leq 0$. This choice is justified by the discussion in §7.

The solution of Config.1 is obtained in terms of $\phi_-(x)$ given in eq. (3.2),

$$\phi_c(x) = \frac{4}{M} \arctan [\exp(-|x - x_i| - c_0)] \quad (4.3)$$

$$= \phi_- (|x - x_i| + c_0), \quad (4.4)$$

where c_0 is the parameter which is determined by the equation,

$$\frac{4}{M} \frac{1}{\cosh(c_0)} + v \sin \left(\chi + \frac{4}{M} \arctan[\exp(-c_0)] \right) = 0. \quad (4.5)$$

This equation is due to the requirement that the jump of the first derivative of $\phi_c(x)$ at x_i should match the third term in the left hand side of eq. (4.1). The solution $\phi_c(x)$ is considered to be a

Fig. 4. The two kinds of the configurations with respect to χ . This figure is for a choice of $M = 4$, $v = 1$ and $\varepsilon = 0$.

kink and an anti-kink connected at the impurity site as shown in Fig. 5. Further the parameter c_0 is equivalent to the distance from the impurity site to the center of the kink as indicated in Fig. 5.

In the case of $\varepsilon \neq 0$, the stable solution, $\phi_s(x)$, in the presence of an impurity given by eq. (4.1) is obtained by the connection at the impurity site of two non-uniform solutions, one of which, $\phi_l(x)$, has been shown in Fig. 2. An example of the stable solution, $\phi_s(x)$, is shown in Fig. 6.

Though the stable solution, $\phi_s(x)$, is obtained only numerically, the information of the phase value at the impurity site is obtained. The stable solution, $\phi_s(x)$, is given as follows;

$$\phi_s(x) = \phi_l(|x - x_i| + c) \quad (4.6)$$

where $\phi_l(x)$ is the non-uniform solution of eq. (3.1) and c is a parameter to be determined to satisfy the boundary condition given by eq. (4.2). When we consider $\phi_s(x)$, it is necessary to consider only the range of solid line in Fig. 6.

Substituting eq. (4.6) into eq. (4.1), we obtain

$$-2\phi'_l(c) + v \sin(\chi + \phi_l(c)) = 0. \quad (4.7)$$

By use of eq. (3.4), eq. (4.7) is rewritten as

$$\left[2 \left[\varepsilon \left(\frac{1}{M} \arcsin(\varepsilon M) - \phi_l(c) \right) + \frac{1}{M^2} \left(\sqrt{1 - (\varepsilon M)^2} - \cos(M\phi_l(c)) \right) \right] \right]^{\frac{1}{2}} + \frac{1}{2}v \sin(\chi + \phi_l(c)) = 0. \quad (4.8)$$

This equation determines the phase value, $\phi_l(c)$, (instead of c) at the impurity site of the stable

Fig. 5. The solid line is the stable solution with an impurity at $x = x_i$ for a choice of $M = 4$, $v = 1$, $\chi = -\pi/M$ and $\varepsilon = 0$.

solution when the electric field, ε , is given. It means that instead of the boundary condition at infinity, eq. (4.2), we obtain a boundary condition at the impurity site.

§5. Threshold Field in the Presence of an Impurity

The depinning threshold field, ε_c , is determined as the field at which the stable solution becomes unstable.⁸⁾ The instability of the solution is triggered by the onset of a zero eigenvalue of the fluctuation mode around the stable solution.⁹⁾

The eigenvalue equation of the fluctuations, $\delta\phi(x)$, around the stable solution, $\phi_s(x)$, is the second variational equation of the Lagrangian; i.e.

$$\left[-\frac{\partial^2}{\partial x^2} + \cos(M\phi_s) + v \cos(\chi + \phi_s) \delta(x - x_i) \right] \delta\phi = \lambda \delta\phi, \quad (5.1)$$

where λ is the eigenvalue. Hence we consider the case of $\lambda = 0$ to determine the threshold field, ε_c .

First, we consider the fluctuation around the solution, $\phi_l(x)$, in the case of $v = 0$. The equation of the zero-mode fluctuation, $\delta\phi_l(x)$, around $\phi_l(x)$ is

$$\left[-\frac{\partial^2}{\partial x^2} + \cos(M\phi_l) \right] \delta\phi_l = 0 \quad (5.2)$$

and the boundary condition is

$$\delta\phi_l(\infty) = 0, \quad \delta\phi'_l(\infty) = 0. \quad (5.3)$$

Its solution is

$$\delta\phi_l(x) \propto \phi'_l(x). \quad (5.4)$$

Fig. 6. The solid line is the stable solution with an impurity for a choice of $M = 4$, $v = 1$, $\chi = -\pi/M$ and $\varepsilon = 0.1$.

Next, we consider the case of $v \neq 0$. The threshold field, ε_c , is determined as a particular value of the electric field at which zero-mode fluctuations in both sides of the impurity are connected. The zero-mode fluctuation around the stable solution in each region must be expressed as

$$\delta\phi(x) \propto -(2\theta(x - x_i) - 1)\phi'_s(x) \quad (5.5)$$

$$= -\phi'_l(|x - x_i| + c), \quad (5.6)$$

by noting

$$\phi'_s(x) = (2\theta(x - x_i) - 1)\phi'_l(x), \quad (5.7)$$

where $\theta(x)$ is the step function. Substituting eq. (5.6) into eq. (5.1), we obtain

$$2\phi''_l(c) - v \cos(\chi + \phi_l(c))\phi'_l(c) = 0. \quad (5.8)$$

At the threshold field, ε_c , eq. (5.8) should be satisfied. By use of eqs. (3.1) and (4.7), eq. (5.8) is expressed as follows;

$$2 \left(-\varepsilon + \frac{1}{M} \sin(M\phi_l(c)) \right) - \frac{1}{4} v^2 \sin[2(\chi + \phi_l(c))] = 0. \quad (5.9)$$

Hence the threshold field, ε_c , is determined as a value of ε at which both eqs. (4.8) and (5.9) have a common solution, $\phi_l(c)$, for each fixed values of χ and v .

The solutions of eqs. (4.8) and (5.9) for $M = 4$ are shown in Fig. 7. The threshold field, ε_c , is normalized by the threshold field, ε_T , of the uniform case. When v is fixed, the normalized

Fig. 7. The threshold field in the presence of an impurity, normalized by that of the uniform case, for a choice of $M = 4$. The threshold field for a choice of $v = 1$ is shown in (a) and for a choice of $\chi = -\pi/M$ is shown in (b).

threshold field goes to 1 as χ tends to $-\pi/(2M)$. It is noted that the threshold field goes to a finite value, ε_∞ , even if $v \rightarrow \infty$. This finite value, ε_∞ , is given by the equation,

$$\varepsilon_\infty \left(\frac{1}{M} \arcsin(\varepsilon_\infty M) + \chi \right) + \frac{1}{M^2} (\sqrt{1 - (\varepsilon_\infty M)^2} - \cos(M\chi)) = 0. \quad (5.10)$$

Through a numerical calculation, we find that for a choice of $\chi = -\pi/M$ and $M = 4$, the normalized threshold field tends to $\varepsilon_\infty/\varepsilon_T \simeq 0.725$ as v tends to infinity.

The reason why $\chi = -\pi/(2M)$ is critical is that $\chi = -\pi/(2M)$ is the value which determines whether the commensurability potential and the impurity potential compete or not at the impurity site, namely, the system contains frustration or not. To investigate the frustration, we consider the local potential energy U_i at the impurity site,

$$U_i(\phi(x_i)) = -\frac{1}{M^2} \cos(M\phi(x_i)) - v \cos(\chi + \phi(x_i)). \quad (5.11)$$

The first term of the right hand is the commensurability potential and the second term is the impurity potential. If the potential energy by the impurity is minimized, that is $\chi + \phi(x_i) = 0$, $U_i(\phi(x_i))$ is

$$U_i(-\chi) = -\frac{1}{M^2} \cos(M\chi) - v. \quad (5.12)$$

In the case of $-\pi/M \leq \chi < -\pi/(2M)$, the commensurability potential and the impurity potential compete and the system contains frustration. In the case of $-\pi/(2M) < \chi \leq 0$, however, they do not compete and the system contains no frustration. When the system is frustrated the effect of the impurity potential to the threshold field is important. However, if the system is not frustrated, the impurity potential is irrelevant.

The reason why the threshold field is finite even if v tends to infinity is that the depinning object is not a particle, but a string. In the limit of $v \rightarrow \infty$ with $\chi = -\pi/M$ which is the optimal case, the cusp of the ground state configuration of the phase is on the top of the barrier of the uniform potential (Fig. 8). The cusp, however, is just a part of the string, and a finite field is necessary for

Fig. 8. The classical solution for a choice of $M = 4$, $\chi = -\pi/M$, $\varepsilon = 0$ and $v \rightarrow \infty$.

a string to go over the uniform potential barrier.

§6. The Potential Curve in the Presence of an Impurity

To clarify the meaning of ε_c , we consider a potential curve in the presence of an impurity. In a homogeneous case the phase is uniform in the ground state, and hence the potential energy density (Fig. 3) can be expressed with respect to the uniform phase variable. With an impurity, however, the phase is not uniform, and therefore we should consider the potential curve in a functional space. In this case the most suitable variable is the phase value, ϕ_i , at the impurity site with χ , v and ε fixed. For each value of ϕ_i , we can determine the lowest energy configuration; we solve eq. (3.1)

under the boundary condition of $\phi(x_i) = \phi_i$ and

$$\phi'(x_i) = - \left[2 \left[\varepsilon \left(\frac{1}{M} \arcsin(\varepsilon M) - \phi_i \right) + \frac{1}{M^2} \left(\sqrt{1 - (\varepsilon M)^2} - \cos(M\phi_i) \right) \right] \right]^{\frac{1}{2}}, \quad (6.1)$$

which is similar to eq. (3.4). Substituting this optimal configuration into eq. (2.2), we determine its energy and obtain the potential curve as the function of ϕ_i which is shown in Fig. 9. While there exists an energy barrier below the threshold field, ε_c , (Fig. 9 (a) and (b)), the barrier disappears at ε_c (Fig. 9 (c)) and CDW depins.

Fig. 9. The potential curve in the presence of an impurity for a choice of $M = 4$, $\chi = -\pi/M$ and $v = 1$; (a) is in the case of $\varepsilon/\varepsilon_c = 0.90$, (b) is in the case of $\varepsilon/\varepsilon_c = 0.98$ and (c) is in the case of $\varepsilon/\varepsilon_c = 1$.

§7. Conclusion and Discussion

We conclude that the existence of an impurity in the model one-dimensional commensurate CDW causes the lowering of threshold fields by a finite amount due to the appearance of the local change of the phase variable, which is considered as nucleation, near an impurity site. Below the threshold field, ε_T , of the uniform depinning, such local change in the homogeneous case always requires a finite excitation energy. However, the nucleation in the presence of an impurity can take place without any excitation energy at field, ε_c , which is smaller than ε_T . The main reason for the lowering of the threshold field is due to the frustration which is caused by the competition between the commensurability potential and the impurity potential.

Our result will be applied to the commensurate CDW with dilute but with macroscopic number of impurities where the inverse of the impurity density is smaller than the phase coherence length, ξ . In such a case these will be a distribution of parameter χ , and then that of the depinning field. However the depinning will be triggered by the nucleation at the optimal impurity site, $\chi = -\pi/M$.

In actual experiments three dimensionality and quantum fluctuations¹⁰⁾ will play important roles at low temperatures, which will be studied elsewhere.

To the best of our knowledge, our investigation is the first microscopic theoretical studies on nucleation triggered by the local inhomogeneity in the bulk region.

Acknowledgments

We would like to thank Hiroshi Kohno for helpful discussions. One of us (M.Y.) is grateful for the kind hospitality received at Condensed Matter Physics Group of Osaka University.

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